

10/ 618,414

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NEWS 5 DEC 14 2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER  
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NEWS 7 DEC 21 IPC search and display fields enhanced in CA/CAPLUS with the  
IPC reform  
NEWS 8 DEC 23 New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/  
USPAT2  
NEWS 9 JAN 13 IPC 8 searching in IFIPAT, IFIUDb, and IFICDB  
NEWS 10 JAN 13 New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to  
INPADOC  
NEWS 11 JAN 17 Pre-1988 INPI data added to MARPAT  
NEWS 12 JAN 17 IPC 8 in the WPI family of databases including WPIFV  
NEWS 13 JAN 30 Saved answer limit increased  
NEWS 14 JAN 31 Monthly current-awareness alert (SDI) frequency  
added to TULSA

NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.  
V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT  
<http://download.cas.org/express/v8.0-Discover/>

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:00:14 ON 07 FEB 2006

=> file reg

10/ 618,414

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:00:56 ON 07 FEB 2006  
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STRUCTURE FILE UPDATES: 6 FEB 2006 HIGHEST RN 873652-66-5  
DICTIONARY FILE UPDATES: 6 FEB 2006 HIGHEST RN 873652-66-5

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

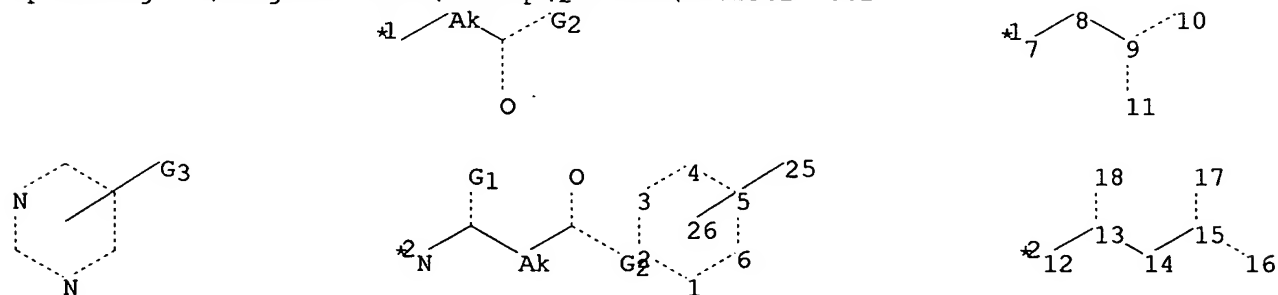
Structure search iteration limits have been increased. See HELP SLIMITS  
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REGISTRY includes numerically searchable data for experimental and  
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experimental property data in the original document. For information  
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=>

Uploading C:\Program Files\Stnexp\Queries\10618414.str



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 25

ring nodes :

1 2 3 4 5 6

chain bonds :

7-8 8-9 9-10 9-11 12-13 13-14 13-18 14-15 15-16 15-17

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ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 8-9 9-10 9-11 12-13 13-14 13-18 14-15  
15-16 15-17

isolated ring systems :

containing 1 :

G1:H,O

G2:O,N

G3:[\*1],[\*2]

Match level :

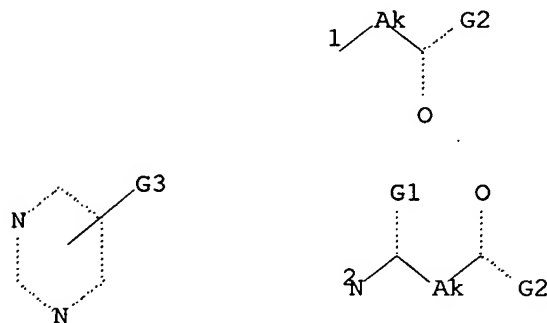
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
25:CLASS 26:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 H,O

G2 O,N

G3 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sample

SAMPLE SEARCH INITIATED 15:01:31 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 80165 TO ITERATE

2.5% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

9 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 1586473 TO 1620127

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PROJECTED ANSWERS: 6075 TO 8353

L2 9 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 15:01:37 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1607858 TO ITERATE

60.7% PROCESSED 975397 ITERATIONS 2650 ANSWERS

62.2% PROCESSED 1000000 ITERATIONS 2663 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.18

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS: 1607858 TO 1607858

PROJECTED ANSWERS: 4085 TO 4477

L3 2663 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
167.38	167.59

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 15:02:16 ON 07 FEB 2006

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FILE COVERS 1907 - 7 Feb 2006 VOL 144 ISS 7

FILE LAST UPDATED: 6 Feb 2006 (20060206/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l3

L4 365 L3

=> s l4 and (nanoic or nanoate)

1 NANOIC

11 NANOATE

L5 0 L4 AND (NANOIC OR NANOATE)

=> s l4 and acid

4097027 ACID

L6 249 L4 AND ACID

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=> s l4 and (nonanoic or nonanoate)

4584 NONANOIC

1650 NONANOATE

L7 9 L4 AND (NONANOIC OR NONANOATE)

=> d his

(FILE 'HOME' ENTERED AT 15:00:14 ON 07 FEB 2006)

FILE 'REGISTRY' ENTERED AT 15:00:56 ON 07 FEB 2006

L1 STRUCTURE UPLOADED

L2 9 S L1 SAMPLE

L3 2663 S L1 FULL

FILE 'CAPLUS' ENTERED AT 15:02:16 ON 07 FEB 2006

L4 365 S L3

L5 0 S L4 AND (NANOIC OR NANOATE)

L6 249 S L4 AND ACID

L7 9 S L4 AND (NONANOIC OR NONANOATE)

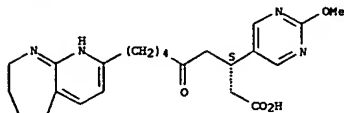
=> d l7 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 9 ANSWERS - CONTINUE? Y/(N):y

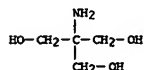
IT 758696-11-2P, [3S]-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(6,7,8,9-tetrahydro-5H-pyrido[2,3-b]azepin-2-yl)nonanoic acid TRIS salt  
RL: IWP (Industrial manufacture); FRP (Properties); SPN (Synthetic preparation); PREZ (Preparation)  
of (target drug; enantioselective process and intermediates for manufacture

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 (methoxypyrimidinyl)oxo(tetrahydropyridoazepinyl)nonanoic  
 acid and analogs, useful as  $\alpha\text{v}\beta 3$  receptor antagonists)  
 RN 758686-11-2 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nanoic acid, 5,6,7,8-tetrahydro- $\beta$ -(2-  
 methoxy-5-pyrimidinyl)-8-oxo-, (8S)-, compd. with  
 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 312262-25-2  
 CMF C23 H30 N4 O4

Absolute stereochemistry. Rotation (-).



CM 2  
 CRN 77-86-1  
 CMF C4 H11 N O3

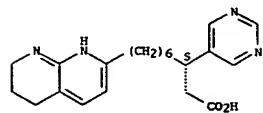


IT 312262-16-1P, (3S)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(5,6,7,8-  
 tetrahydro-1,8-naphthyridin-2-yl)nonanoic acid  
 758686-12-3P, (3S)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(5,6,7,8-  
 tetrahydro-1,8-naphthyridin-2-yl)nonanoic acid TRIS salt  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
 (Preparation)  
 of (target drug; enantioselective process and intermediates for manufacture  
 (methoxypyrimidinyl)oxo(tetrahydropyridoazepinyl)nonanoic  
 acid and analogs, useful as  $\alpha\text{v}\beta 3$  receptor antagonists)  
 RN 312262-16-1 CAPLUS  
 CN 1,8-Naphthyridine-2-nanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methoxy-5-  
 pyrimidinyl)-8-oxo-, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

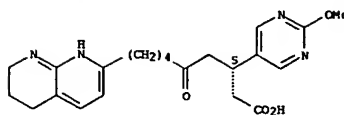
L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:694278 CAPLUS  
 DOCUMENT NUMBER: 141:325163  
 TITLE: Nonpeptide  $\alpha\text{v}\beta 3$  Antagonists. Part 11:  
 Discovery and Preclinical Evaluation of Potent  
 $\alpha\text{v}\beta 3$  Antagonists for the Prevention and  
 Treatment of Osteoporosis  
 AUTHOR(S): Coleman, Paul J.; Brashear, Karen M.; Askew, Ben C.;  
 Hutchinson, John H.; McVean, Carol A.; Duong, Le T.;  
 Feuston, Bradley P.; Fernandez-Metzler, Carmen;  
 Gentile, Michael A.; Hartman, George D.; Kimmel,  
 Donald B.; Leu, Chih-Tai; Lipfert, Lorraine; Meckle,  
 Kara; Pennypacker, Brenda; Prueksaritanont, Thomayant;  
 Rodan, Gideon A.; Wesolowski, Gregg A.; Rodan, Sevil  
 B.; Duggan, Mark E.  
 CORPORATE SOURCE: Departments of Medicinal Chemistry, Bone Biology and  
 Osteoporosis Research, Drug Metabolism and Pharmacology  
 and Molecular Systems, Merck Research Laboratories,  
 West Point, PA, 19486, USA  
 SOURCE: Journal of Medicinal Chemistry (2004), 47(20),  
 4829-4837  
 CODEN: JMCMAH; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 141:325163  
 AB 3-(S)-Pyrimidin-5-yl-9-(5,6,7,8-tetrahydro-[1,8]naphthyridin-2-yl)-  
 nonanoic acid (5e) and 3-(S)-(methylpyrimidin-5-yl)-9-(5,6,7,8-  
 tetrahydro-[1,8]naphthyridin-2-yl)-nonanoic acid (5f) were  
 identified as potent and selective antagonists of the  $\alpha\text{v}\beta 3$   
 receptor. These compds. have excellent in vitro profiles (IC<sub>50</sub> = 0.07 and  
 0.08 nM, resp.), significant unbound fractions in human plasma (6 and 4%),  
 and good pharmacokinetics in rat, dog, and rhesus monkey. On the basis of  
 the efficacy shown in an in vivo model of bone turnover following  
 once-daily oral administration, these two compds. were selected for clin.  
 development for the treatment of osteoporosis.  
 IT 227752-24-1P 227753-49-3P 227753-52-8P  
 769936-46-1P  
 RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP  
 (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL  
 (Biological study); PREP (Preparation); USES (Uses)  
 (nonpeptide  $\alpha\text{v}\beta 3$  antagonists in discovery and preclin.  
 evaluation of potent  $\alpha\text{v}\beta 3$  antagonists for prevention and  
 treatment of osteoporosis)  
 RN 227752-24-1 CAPLUS  
 CN 1,8-Naphthyridine-2-nanoic acid, 1,5,6,7-tetrahydro- $\beta$ -5-pyrimidinyl-  
 -, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 227753-49-3 CAPLUS

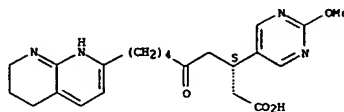
L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



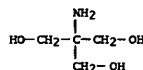
RN 758686-12-3 CAPLUS  
 CN 1,8-Naphthyridine-2-nanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methoxy-5-  
 pyrimidinyl)-8-oxo-, (8S)-, compd. with 2-amino-2-  
 (hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1  
 CRN 312262-16-1  
 CMF C22 H28 N4 O4

Absolute stereochemistry.

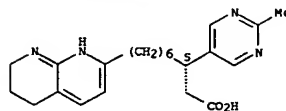


CM 2  
 CRN 77-86-1  
 CMF C4 H11 N O3



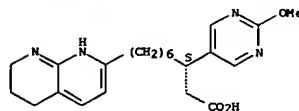
L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 CN 1,8-Naphthyridine-2-nanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-  
 pyrimidinyl)-, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



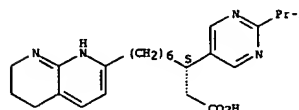
RN 227753-52-8 CAPLUS  
 CN 1,8-Naphthyridine-2-nanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-  
 pyrimidinyl)-, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 769936-46-1 CAPLUS  
 CN 1,8-Naphthyridine-2-nanoic acid, 1,5,6,7-tetrahydro- $\beta$ -[2-(1-  
 methylethyl)-5-pyrimidinyl]-, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

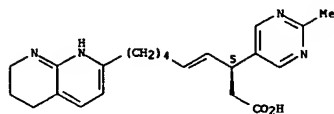


IT 769936-69-8P 769936-70-1P 769936-71-2P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (nonpeptide  $\alpha\text{v}\beta 3$  antagonists in discovery and preclin.  
 evaluation of potent  $\alpha\text{v}\beta 3$  antagonists for prevention and  
 treatment of osteoporosis)

RN 769936-69-8 CAPLUS  
 CN 5-Pyrimidinopropanoic acid, 2-methyl- $\beta$ -[6-(1,5,6,7-tetrahydro-1,8-  
 naphthyridin-2-yl)-1-hexenyl]-, (8S)- (9CI) (CA INDEX NAME)

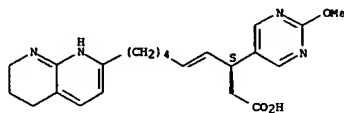
Absolute stereochemistry.  
 Double bond geometry unknown.

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



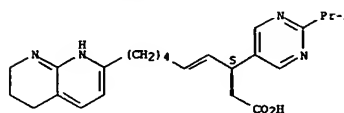
RN 769936-70-1 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, 2-methoxy-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.



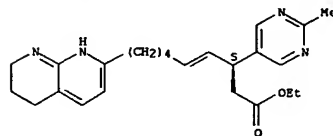
RN 769936-71-2 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, 2-(1-methylethyl)-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.



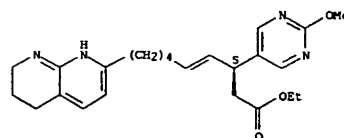
IT 227752-22-9P 769936-34-7P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (nonpeptide  $\alpha\text{v}\beta 3$  antagonists in discovery and preclin. evaluation of potent  $\alpha\text{v}\beta 3$  antagonists for prevention and treatment of osteoporosis)  
 RN 227752-22-9 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, ethyl ester, (BS)- (9CI) (CA INDEX NAME)

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



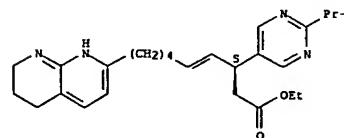
RN 769936-64-3 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, 2-methoxy-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.

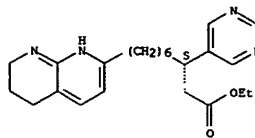


RN 769936-65-4 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, 2-(1-methylethyl)-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.

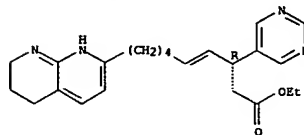


REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 Absolute stereochemistry.

RN 769936-34-7 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.



IT 431040-43-6P 769936-64-3P 769936-65-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (nonpeptide  $\alpha\text{v}\beta 3$  antagonists in discovery and preclin. evaluation of potent  $\alpha\text{v}\beta 3$  antagonists for prevention and treatment of osteoporosis)  
 RN 431040-43-6 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (BS)- (9CI) (CA INDEX NAME)

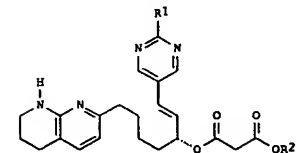
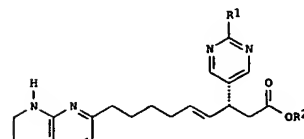
Absolute stereochemistry.  
 Double bond geometry unknown.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:696685 CAPLUS  
 DOCUMENT NUMBER: 139:230784  
 TITLE: Malonate-Claisen rearrangement for preparation of integrin receptor antagonist intermediates  
 INVENTOR(S): Humphrey, Guy R.; Farr, Roger N.; Lee, Jaemoon  
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA  
 SOURCE: PCT Int. Appl., 25 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072042	A2	20030904	WO 2003-US5476	20030221
WO 2003072042	A3	20040304		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZH, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 PRIORITY APPLN. INFO.: US 2002-360273P P 20020227  
 OTHER SOURCE(S): CASREACT 139:230784; MARPAT 139:230784  
 GI

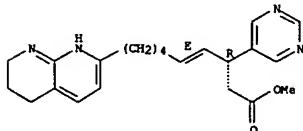


AB A process is described for the preparation of chiral unsatd. ester

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
intermediates [I: having the (R)-configuration at the stereogenic center marked with \*R] = H, methyl; R2 = Cl-4 alkyl, phenyl-Cl-3-alkyl; e.g., 3-(R)-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)-(E)-non-4-enoic acid Me ester], useful in the asym. syntheses of  $\alpha$ v $\beta$ 3 integrin receptor antagonists (no data), which involves an efficient Claisen rearrangement of a malonate ester of a chiral allylic alc. precursor [II: e.g., Et malonate ester of (R)-1-(pyrimidin-5-yl)-7-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)-(E)-hept-1-en-3-ol] followed by hydrolysis and decarboxylation. The unsatd. ester intermediates can be converted in a 2-step sequence into the desired substituted nonanoic acid deriva. [e.g., 3-(S)-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)nonanoic acid Me ester].

IT 593282-80-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(in a malonate-Claisen rearrangement for preparation of integrin receptor antagonist intermediates)  
RN 593282-80-5 CAPLUS  
CN 5-Pyrimidinepropanoic acid,  $\beta$ -{[(E)-6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, methyl ester, (RR)- (9CI) (CA INDEX NAME)

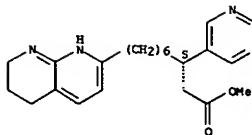
Absolute stereochemistry.  
Double bond geometry as shown.



IT 593282-81-6P 593282-82-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(malonate-Claisen rearrangement for preparation of integrin receptor antagonist intermediates)  
RN 593282-81-6 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -5-pyrimidinyl-, methyl ester, (BS)- (9CI) (CA INDEX NAME)

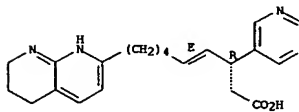
Absolute stereochemistry.

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



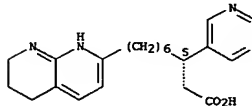
RN 593282-82-7 CAPLUS  
CN 5-Pyrimidinepropanoic acid,  $\beta$ -{[(E)-6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, (RR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



IT 227752-24-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(malonate-Claisen rearrangement for preparation of integrin receptor antagonist intermediates)  
RN 227752-24-1 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -5-pyrimidinyl-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2002:977654 CAPLUS

DOCUMENT NUMBER: 138:61306

TITLE: Preparation of pharmaceuticals containing  
(pyrimidinyl)tetrahydronaphthyridinylnonanoic acid  
This salt as an integrin receptor antagonist  
Humphrey, Guy R.; Xu, Wei  
Merk & Co., Inc., USA  
PCT Int. Appl., 21 pp.  
CODEN: PIXX02

DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002102374	A1	20021227	WO 2002-US18906	20020614
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZH, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CA, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, CR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003004171	A1	20030102	US 2002-174016	20020618
US 6750220	B2	20040615	US 2001-299344P	P 20010619

PRIORITY APPL. INFO.:  
AB The tris(hydroxymethyl)aminomethane ("TRIS") salt of 3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)nonanoic acid is a potent antagonist of the integrin  $\alpha$ v $\beta$ 3 receptor and is useful for the prevention and/or treatment of osteoporosis and vascular restenosis, as well as conditions associated with excessive angiogenesis, such as macular degeneration, diabetic retinopathy, atherosclerosis, inflammatory arthritis, cancer, and metastatic tumor growth. The invention also relates to a process for the preparation of the salt as well

as pharmaceutical compns. containing the salt and methods of using the salt. Thus, the 3R or 3S isomer of 3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)nonanoic acid was treated with tris(hydroxymethyl)aminomethane in EtOH solution to give the title salts. The products were characterized by x-ray diffraction and FT-IR spectra and DSC. A 100-mg tablet is composed of 133 mg the active ingredient, 243 mg lactose, 20 mg croscarmellose sodium, and 4 mg magnesium stearate.

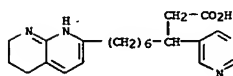
IT 479063-88-2P 479063-89-6P 479063-90-6P 479063-91-9P  
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of pharmaceuticals containing  
(pyrimidinyl)tetrahydronaphthyridinyl  
nonanoic acid Tris salt as integrin receptor antagonist)

RN 479063-88-2 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -5-pyrimidinyl-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CH 1

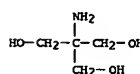
CRN 227753-43-7  
CMF C21 H28 N4 O2

L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CH 2

CRN 77-86-1  
CMF C4 H11 N O3

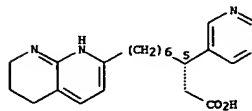


RN 479063-90-6 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -5-pyrimidinyl-, (BS)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CH 1

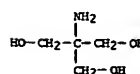
CRN 227752-24-1  
CMF C21 H28 N4 O2

Absolute stereochemistry.



CH 2

CRN 77-86-1  
CMF C4 H11 N O3



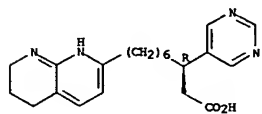
RN 479063-93-9 CAPLUS

L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -5-pyrimidinyl-, (BR)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

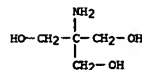
CRN 227752-23-0  
 CMF C21 H28 N4 O2

Absolute stereochemistry.



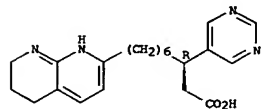
CM 2

CRN 77-86-1  
 CMF C4 H11 N O3



IT 227752-23-0 227752-24-1 227753-43-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of pharmaceuticals containing  
 (pyrimidinyl)tetrahydronaphthyridinyl  
 nonanoic acid Tris salt as integrin receptor antagonist)  
 RN 227752-23-0 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -5-pyrimidinyl-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:409266 CAPLUS  
 DOCUMENT NUMBER: 136:409377  
 TITLE: Preparation of amine salts of an integrin receptor antagonist  
 INVENTOR(S): Humphrey, Guy R.; Waters, Marjorie See; Xu, Wei  
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA  
 SOURCE: U.S. Pat. Appl. Publ., 21 pp.  
 CODEN: USKXCD  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002065291	A1	20020530	US 2001-998416	20011129
US 6444680	B2	20020903		

PRIORITY APPLN. INFO.: US 2000-250268P P 20001130  
 AB Amine salts of 3-(2-methyl-pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-[1,8]-naphthyridin-2-yl)nonanoic acid are potent antagonists of the integrin  $\alpha v \beta 3$  receptor and are useful for the prevention and/or treatment of osteoporosis and vascular restenosis, as well as conditions associated with excessive angiogenesis, such as macular degeneration, diabetic retinopathy, atherosclerosis, inflammatory arthritis, cancer, and metastatic tumor growth. The invention also relates to a process for the preparation of the novel salts as well as pharmaceutical compns. containing

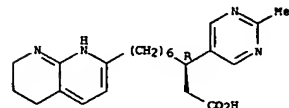
the salts and methods of using the salts. Also disclosed are 3(R)- and 3(S)-[2-methylpyrimidin-5-yl]-9-(5,6,7,8-tetrahydro-[1,8]naphthyridin-2-yl)nonanoic acid (I) in the form of a zwitterion trihydrate. Thus, I were prepared in a series of steps. A 100-mg tablet was composed of 100 mg active ingredient, 276 mg mannitol, 20 mg of croscarmellose sodium, and 4 mg magnesium stearate.

IT 431040-45-8P 431040-46-9P 431040-47-0P  
 431040-48-1P 431040-49-2P 431040-50-5P  
 RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of amine salts of integrin receptor antagonist)  
 RN 431040-45-8 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)-, (BR)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

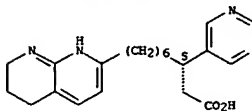
CRN 227753-48-2  
 CMF C22 H30 N4 O2

Absolute stereochemistry.

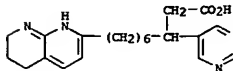


L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 RN 227752-24-1 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -5-pyrimidinyl-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 227753-43-7 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -5-pyrimidinyl-, (9CI) (CA INDEX NAME)

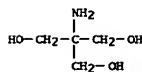


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 77-86-1  
 CMF C4 H11 N O3

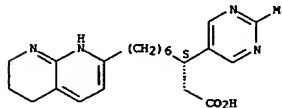


RN 431040-46-9 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)-, (BS)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

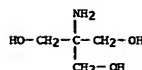
CRN 227753-49-3  
 CMF C22 H30 N4 O2

Absolute stereochemistry.



CM 2

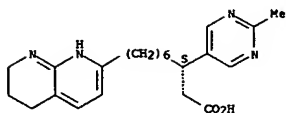
CRN 77-86-1  
 CMF C4 H11 N O3



RN 431040-47-0 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)-, trihydrate, (BS)- (9CI) (CA INDEX NAME)

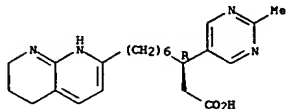
Absolute stereochemistry.

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● 3 H<sub>2</sub>O

RN 431040-48-1 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, trihydrate, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

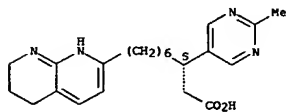
● 3 H<sub>2</sub>O

RN 431040-49-2 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (BS)-, compd. with 2-amino-2-methyl-1-propanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 227753-49-3  
 CMF C22 H30 N4 O2

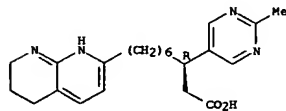
Absolute stereochemistry.



L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

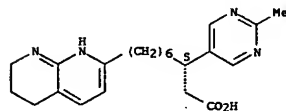
RN 227753-48-2 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



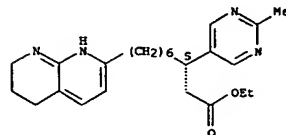
RN 227753-49-3 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 404869-67-6 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



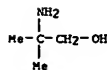
RN 431040-42-5 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 124-68-5  
 CMF C4 H11 N O

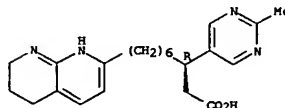


RN 431040-50-5 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (BR)-, compd. with 2-amino-2-methyl-1-propanol (1:1) (9CI) (CA INDEX NAME)

CM 1

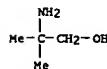
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 CMF C22 H30 N4 O2

Absolute stereochemistry.



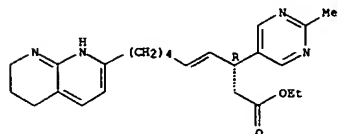
CM 2

CRN 124-68-5  
 CMF C4 H11 N O



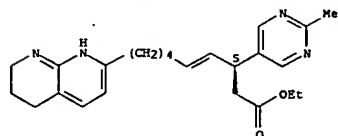
IT 227753-48-2P 227753-49-3P 404869-67-6P  
 431040-42-5P 431040-43-6P 431040-44-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of amine salts of integrin receptor antagonist)

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



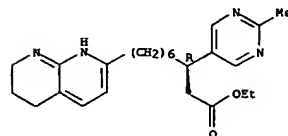
RN 431040-43-6 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.



RN 431040-44-7 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

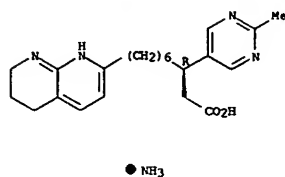


IT 431040-51-6P 431040-52-7P 431040-53-8P  
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of amine salts of integrin receptor antagonist)  
 RN 431040-51-6 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, monoammonium salt, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

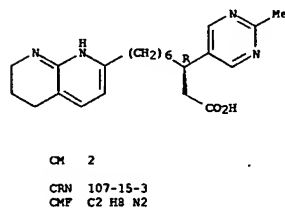
10/ 618,414

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 431040-52-7 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (8R)-, compd. with 1,2-ethanediamine (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 227753-48-2  
 CMF C22 H30 N4 O2

Absolute stereochemistry.



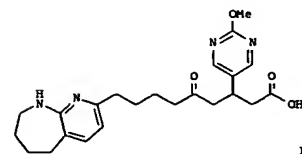
H2N-CH2-CH2-NH2

RN 431040-53-8 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (8R)-, compd. with N-(phenylmethyl)benzenemethanamine (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 227753-48-2  
 CMF C22 H30 N4 O2

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 ACCESSION NUMBER: 2002:275794 CAPLUS  
 DOCUMENT NUMBER: 136:309803  
 TITLE: Preparation of a phosphoric acid salt of an integrin receptor antagonist  
 INVENTOR(S): Weissenberger, Robert S.; Xu, Wei  
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA  
 SOURCE: PCT Int. Appl., 27 pp.  
 CODEN: PIXX02  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002028395	A1	20020411	WO 2001-US30647	20011001
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2424117	AA	20020411	CA 2001-2424117	20011001
AU 2001096439	A5	20020415	AU 2001-96439	20011001
EP 1326615	A1	20030716	EP 2001-977309	20011001
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, UK, CY, AL, TR				
JP 2004510738	T2	20040408	JP 2002-532220	20011001
US 2005101593	A1	20050512	US 2003-398366	20011001
PRIORITY APPLN. INFO.:				
US 2000-237534P				
WO 2001-US30647				
P 20001004				
W 20011001				

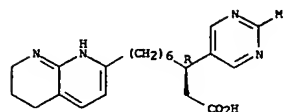
GI



AB The phosphoric acid salt of 3-[2-methoxy-pyrimidin-5-yl]-5-oxo-9-(6,7,8,9-tetrahydro-5H-pyrido[2,3-b]azepin-2-yl)-nonanoic acid (I) is a potent antagonist of the integrin αvβ3 receptor and is useful for the prevention and/or treatment of osteoporosis and vascular restenosis, as well as conditions associated with excessive angiogenesis, such as macular degeneration, diabetic retinopathy, atherosclerosis, inflammatory arthritis, cancer, and metastatic tumor growth. The

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

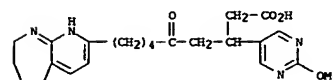
Absolute stereochemistry.



CM 2  
 CRN 103-49-1  
 CMF C14 H15 N

Ph-CH2-NH-CH2-Ph

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 invention also relates to a process for the prepn. of the novel salt as well as pharmaceutical compns. and methods of use. Thus, I·H3PO4 was prepd. from I Et ester via sapon. with aq. NaOH followed by reaction of H3PO4 in EtOH. The the crystal structure of I·H3PO4 was datd. via x-ray powder diffraction.  
 IT 408357-11-9P 408357-12-0P 408357-13-1P  
 RI: PRP (Properties); SPN (Synthetic preparation); THRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of crystalline phosphoric acid salt of integrin αvβ3 receptor antagonist useful as therapeutic for osteoporosis and vascular restenosis)  
 RN 408357-11-9 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-5-oxo-, phosphate (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 312262-23-0  
 CMF C23 H30 N4 O4



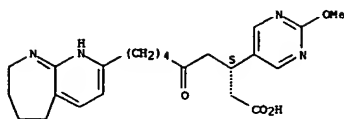
CM 2  
 CRN 7664-38-2  
 CMF H3 O4 P



RN 408357-12-0 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-5-oxo-, (8S)-, phosphate (1:1) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 312262-25-2  
 CMF C23 H30 N4 O4

Absolute stereochemistry. Rotation (-).

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

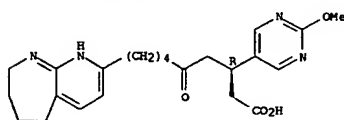
CRN 7664-38-2  
CMF H3 O4 P

RN 408357-13-1 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (BR)-, phosphate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 312262-24-1  
CMF C23 H30 N4 O4

Absolute stereochemistry.

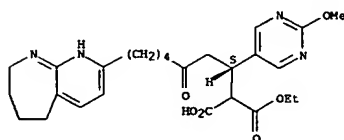


CM 2

CRN 7664-38-2  
CMF H3 O4 P

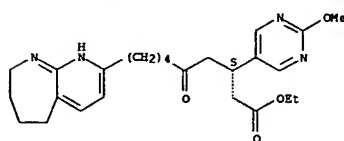
L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



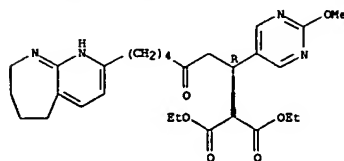
RN 408357-21-1 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, ethyl ester, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 408357-23-3 CAPLUS  
CN Propanedioic acid, [(1R)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



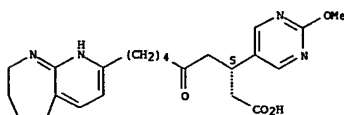
IT 312262-23-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of crystalline phosphoric acid salt of integrin αvβ3 receptor antagonist useful as therapeutic for osteoporosis and vascular restenosis)  
RN 312262-23-0 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



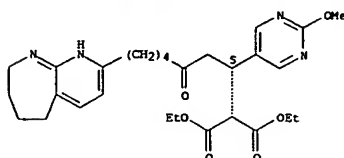
IT 312262-25-2P 408357-19-7P 408357-20-0P  
408357-21-1P 408357-23-3P  
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of crystalline phosphoric acid salt of integrin αvβ3 receptor antagonist useful as therapeutic for osteoporosis and vascular restenosis)  
RN 312262-25-2 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 408357-19-7 CAPLUS  
CN Propanedioic acid, [(1S)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

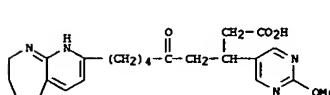
Absolute stereochemistry.



RN 408357-20-0 CAPLUS  
CN Propanedioic acid, [(1S)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, monoethyl ester (9CI) (CA INDEX NAME)

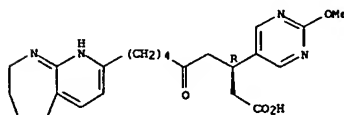
L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

methoxy-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)

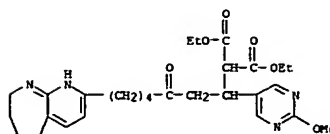


IT 312262-24-1P 408357-18-6P 408357-25-5P  
408357-27-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of crystalline phosphoric acid salt of integrin αvβ3 receptor antagonist useful as therapeutic for osteoporosis and vascular restenosis)  
RN 312262-24-1 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

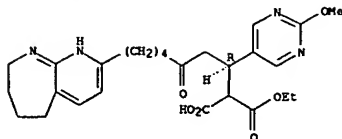


RN 408357-18-6 CAPLUS  
CN Propanedioic acid, [1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)



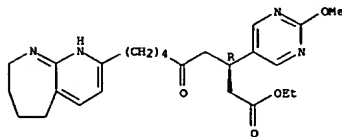
RN 408357-25-5 CAPLUS  
CN Propanedioic acid, [(1R)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, monoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



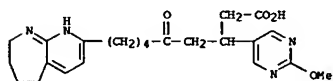
RN 408357-27-7 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-β-oxo-, ethyl ester, (βR) - (9CI) (CA INDEX NAME)

**Absolute stereochemistry.**



IT 312262-23-ODP, salt  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of crystalline phosphoric acid salt of integrin  $\alpha v \beta 3$   
receptor antagonist useful as therapeutic for osteoporosis and vascular  
diseases)

RN 312262-23-0 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro- $\beta$ -(2-methoxy-5-pyrimidinyl)-8-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS ON STN (Continued)  
alkyl, C1-6 alkoxyl, C1-4 alkoxy-C1-6 alkyl, hydroxycarbonyl,  
hydroxycarbonyl-C1-6 alkyl, C1-3 alkoxycarbonyl, C1-3 alkoxycarbonyl-C1-6  
alkyl, hydroxy, hydroxy-C1-6-alkyl, nitro, cyano, trifluoromethyl,  
trifluoromethoxy, trifluoroethoxy, C1-8 alkyl-S(=O)(0-2, C1-8  
alkyl)0-2-aminocarbonyl, C1-8 alkoxycarbonylaminocarbonyl, (C1-8  
alkyl)1-2-aminocarbonyloxy, (aryl C1-3 alkyl)1-2-amino, (aryl)1-2-amino,  
aryl-C1-3 alkylsulfonylaminocarbonyl, and C1-8 alkylsulfonylaminocarbonyl or two R1  
substituents, when on the same nonarom. C atom, are taken together with  
the C atom to which they are attached to form a carbonyl group, or two R1  
substituents, together with the nonarom. C atom to which they are attached,  
attached, join to form a 4- to 6-membered satd. or unsatd. carbocyclic  
ring. R2 is H or C1-4 alkyl; R3 is fluoro and R4 is H or R3 is H and R4  
is fluoro. Although the methods of prepn. are not claimed, .apprx.10  
example preps. are included. Representative compds. of the present  
invention were tested and found to bind to human  $\alpha v \beta 3$  integrin.  
These compds. were generally found to have IC50 values  $<10$  nM in the SPAPV3  
assay. Representative compds. of the present invention were also tested  
in the SPAPV5 assay to det. affinity for the  $\alpha v \beta 5$  receptor.

IT 321262-91-25, (2-[1,8-naphthyridin-2-yl]naphthalen-5-yl) 3-oxo-7-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)heptyl]nonanoic acid diethyl ester 312262-95-6P, 3-(2-Methylpyrimidin-5-yl)pent-4-enoic acid ethyl ester 312262-96-7P, 5-Hydroxy-3-(2-methylpyrimidin-5-yl)pentanoic acid ethyl ester 312262-97-8P, 3-(2-Methylpyrimidin-5-yl)-5-oxopentanoic acid ethyl ester 312263-52-8P, 2-[(1S)-[2-methylpyrimidin-5-yl]-3-oxo-7-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)naphthalen-5-yl]nonanoic acid diethyl ester 393177-66-7P, (3S)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-67-8P, (3S)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-69-0P, (3R)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-69-1P, (3S)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(3-cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-72-5P, (3R)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(3-cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-73-6P, (3S)-9-(3-Cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-5,5-difluoro-3-(2-methylpyrimidin-5-yl)nonanoic acid ethyl ester 393177-76-9P, (3S)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-77-0P, (3R)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-78-1P, (3S)-5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-80-5P, (3S)-3-(2-Methoxypyrimidin-5-yl)-4-(2-[4-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)butyl]-1,3-dithioan-2-yl)butanoic acid ethyl ester 393177-81-8P, (3S)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(3-bromo-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-82-7P, 3-(2-Methylpyrimidin-5-yl)-7-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-86-1P, 3-(2-Methylpyrimidin-5-yl)-7-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-non-5-enoic acid ethyl ester 393177-87-2P, (3S)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-10-yl)nonanoic acid ethyl ester 393177-89-3P, (3R)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-10-yl)nonanoic acid ethyl ester

RL: RCT (Reactant); SPN (Synthetic Preparation); PREP (Preparation); RAC

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS ON STN  
ACCESSION NUMBER: 2002:89834 CAPLUS  
DOCUMENT NUMBER: 136:134745  
TITLE: Preparation of heterocycle-substituted  
chain-fluorinated carboxylic acids and esters useful  
as av integrin receptor antagonists  
INVENTOR(S): Wang, Jiabing  
PATENT ASSIGNEE(S): Merck & Co., Inc., USA  
SOURCE: PCT Int. Appl., 98 pp.  
CODEN: PIXX02  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002007730	A1	20020131	WO 2001-US22938	20010720
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, IL, IN, IS, JP, KZ, KG, KR, LC, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SZ, SI, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, CA, BF, CG, CI, CM, CA, GN, GO, GW, ML, HR, NE, SN, TO, TG			
CA 146751	A	20020131	CA 2001-2416751	20010720
AU 2001077935	AA	20020205	AU 2001-77935	20010720
EP 1315501	A1	20020604	EP 2001-955884	20010720
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, IL, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, LR, TR, LT, LU, NL, SE, MC, PT,			
JP 2004504349	T2	20040212	JP 2002-513465	20010720
US 2004038963	A1	20040226	US 2002-276048	20021112
PRIORITY APPLN. INFO.:			US 2000-220903P	P 20000726
			WO 2001-US22938	WO 20010720

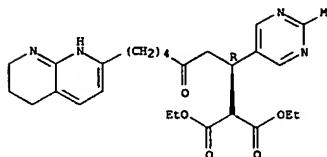
OTHER SOURCE(S): MARPAT 136:134745

AB The present invention relates to novel chain-fluorinated alkanonic acid derivs. XCH<sub>2</sub>CH<sub>2</sub>C-CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>R6 [1, e.g. (3S)-5,5-difluoro-3-(2-methylpropyl)-5-yl]-9- (5,6,7,8-tetrahydro[1,8-naphthalen-2-yl) nonanoic acid), their synthesis, and their use as  $\alpha$ v integrin receptor antagonists. More particularly, the compds. of the present invention are antagonists of the integrin receptors  $\alpha$ v $\beta$ 3 and/or  $\alpha$ v $\beta$ 5 and are useful for inhibiting bone resorption, treating and preventing osteoporosis, and inhibiting vascular restenosis, diabetic retinopathy, macular degeneration, angiogenesis, atherosclerosis, inflammation, inflammatory arthritis, viral disease, cancer, and metastatic tumor growth. In 1, X = 5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl, 2,3-dihydro-1,8-bipyrido[2,3-b]pyridin-2-yl, 5,6,7,8-tetrahydro-9H-pyrido[1,2-b]pyrazole-2,3-yl, or 6-R<sub>2</sub>NHpyridin-2-yl, where each R<sub>2</sub> atom is a ring atom or a substituent atom independently substituted with one or two p-RI substituents and each aromatic ring atom is unsubstituted with one or two p-RI substituents and each aromatic ring atom is substituted with one or two p-RI substituents with one RI substituent. RI = C1-8 alkyl, C3-8 cycloalkyl, C3-8 cycloheteroalkyl, C3-8 cycloalkyl-C1-6 alkyl, C3-8 cycloheteroalkyl-C1-6 alkyl, aryl, aryl-C1-6 alkyl, amino, amino-C1-6 alkyl, C3-8 acylamino, C1-3 acylamino-C1-6 alkyl, (C1-6 alkyl)-1-2-amino, C3-6 cycloalkyl-CO-2 amino, (C1-6 alkyl)-1-2-amino-C1-6

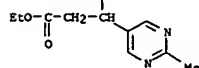
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
(Reactant or reagent)  
(intermediate; prepn. of heterocycle-substituted chain-fluorinated  
carboxylic acids and esters useful as av integrin receptor  
antagonists)

RN 312262-91-2 CAPLUS  
CN Propanedioic acid, [(1R)-1-(2-methyl-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

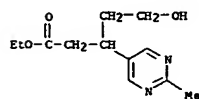
### Absolute stereochemistry.



RN 312262-95-6 CAPLUS  
CN 5-Pyrimidinepropanoic acid,  $\beta$ -ethenyl-2-methyl-, ethyl ester (9CI)  
(CA INDEX NAME)

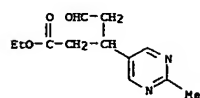


RN 312262-96-7 CAPLUS  
CN 5-Pyrimidinepropanoic acid,  $\beta$ -(2-hydroxyethyl)-2-methyl-, ethyl ester  
(9CI) (CA INDEX NAME)



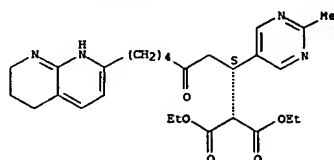
RN 312262-97-8 CAPLUS  
CN 5-Pyrimidinepropanoic acid, 2-methyl- $\beta$ -(2-oxoethyl)-, ethyl ester  
(9CI) (CA INDEX NAME)

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



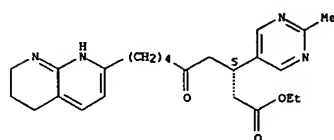
RN 312263-52-8 CAPLUS  
 CN Propanedioic acid, [(1S)-1-(2-methyl-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393177-66-7 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-8-oxo-, ethyl ester, (8S)- (9CI) (CA INDEX NAME)

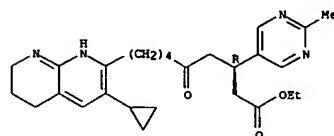
Absolute stereochemistry.



RN 393177-67-8 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 5,8-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (8S)- (9CI) (CA INDEX NAME)

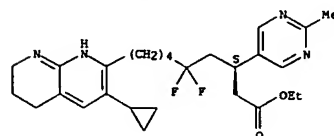
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



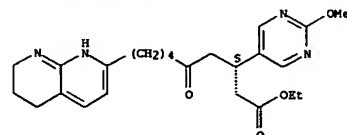
RN 393177-73-6 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-5,8-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393177-76-9 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-8-oxo-, ethyl ester, (8S)- (9CI) (CA INDEX NAME)

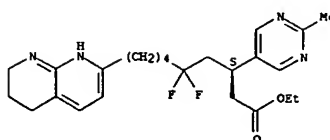
Absolute stereochemistry.



RN 393177-77-0 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-8-oxo-, ethyl ester, (8R)- (9CI) (CA INDEX NAME)

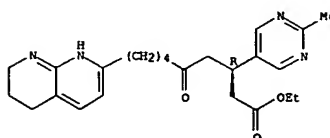
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



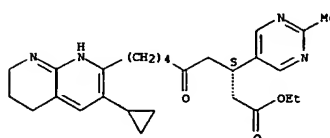
RN 393177-69-0 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-8-oxo-, ethyl ester, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393177-71-4 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-8-oxo-, ethyl ester, (8S)- (9CI) (CA INDEX NAME)

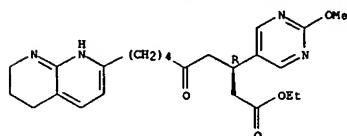
Absolute stereochemistry.



RN 393177-72-5 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-8-oxo-, ethyl ester, (8R)- (9CI) (CA INDEX NAME)

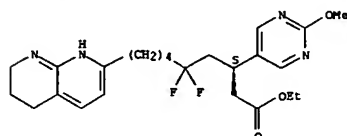
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



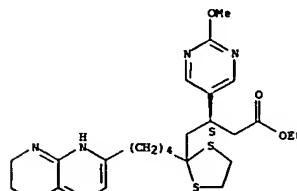
RN 393177-78-1 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 5,8-difluoro-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, ethyl ester, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



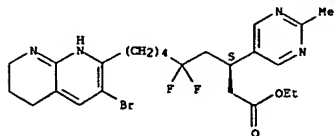
RN 393177-80-5 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, 2-methoxy-β-[[2-(4-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)butyl)-1,3-dithiolan-2-yl]methyl]-, ethyl ester, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

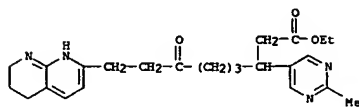


RN 393177-81-6 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 3-bromo-5,8-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (8S)- (9CI) (CA INDEX NAME)

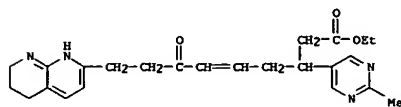
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
Absolute stereochemistry.



RN 393177-82-7 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-ζ-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 393177-86-1 CAPLUS  
CN 5-Pyrimidinopropanoic acid, 2-methyl-β-[4-oxo-6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-2-hexenyl]-, ethyl ester (9CI) (CA INDEX NAME)



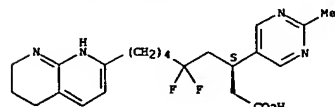
RN 393177-87-2 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
2-yl)-5,5-difluoro-3-(2-methylpyrimidin-5-yl)nonanoic acid  
393177-95-2P, 5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid  
393177-96-3P, (3S)-5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid  
393177-97-4P, (3R)-5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid  
393177-98-5P, 5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid  
393177-99-6P, (3S)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid  
393178-00-2P, (3R)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid  
393178-01-3P, 5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid  
393178-02-4P, (3S)-5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid  
393178-03-5P, (3R)-5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid  
RU: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of heterocycle-substituted chain-fluorinated carboxylic acids and esters useful as ev integrin receptor antagonists)

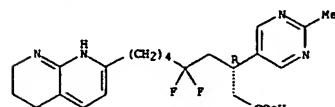
RN 393177-64-5 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



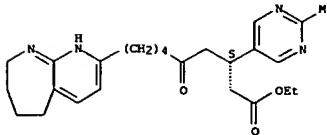
RN 393177-68-9 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



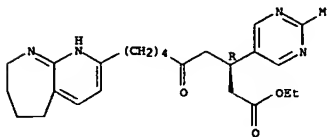
RN 393177-70-3 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-δ,δ-difluoro-

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 393177-88-3 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

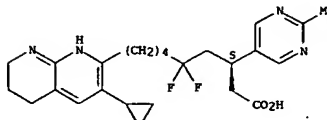
Absolute stereochemistry.



IT 393177-64-5P, (3S)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid  
393177-68-9P, (3R)-5,5-Difluoro-3-(2-Methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid  
393177-70-3P, (3S)-9-(3-Cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-5,5-difluoro-3-(2-methylpyrimidin-5-yl)nonanoic acid  
393177-74-7P, (3R)-9-(3-Cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-5,5-difluoro-3-(2-methylpyrimidin-5-yl)nonanoic acid  
393177-75-8P, (3S)-5,5-Difluoro-3-(2-Methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid  
393177-79-2P, (3R)-5,5-Difluoro-3-(2-Methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid  
393177-89-4P, 5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid  
393177-90-7P, (3S)-5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid  
393177-91-8P, (3R)-5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid  
393177-92-9P, 5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid  
393177-93-0P, 5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid  
393177-94-1P, 9-(3-Cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-

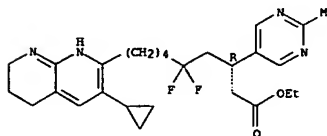
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



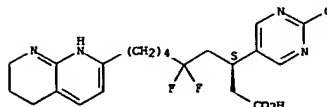
RN 393177-74-7 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393177-75-8 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, (R)- (9CI) (CA INDEX NAME)

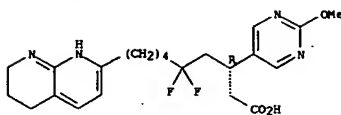
Absolute stereochemistry.



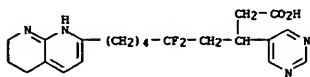
RN 393177-79-2 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

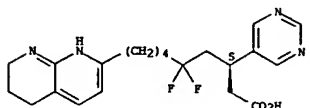


RN 393177-89-4 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 8,8-difluoro-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



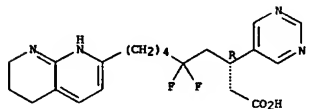
RN 393177-90-7 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 8,8-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



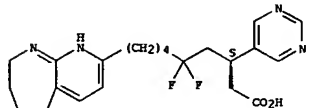
RN 393177-91-8 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 8,8-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



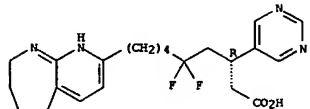
RN 393177-92-9 CAPLUS

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

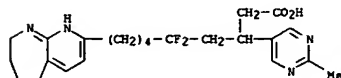


RN 393177-97-4 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 8,8-difluoro-5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

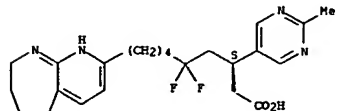


RN 393177-98-5 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 8,8-difluoro-5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (8S)- (9CI) (CA INDEX NAME)



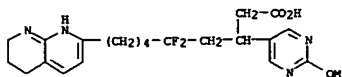
RN 393177-99-6 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 8,8-difluoro-5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

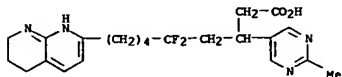


RN 393178-00-2 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 8,8-difluoro-5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (8R)- (9CI) (CA INDEX NAME)

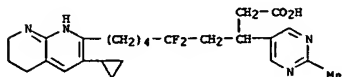
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 CN 1,8-Naphthyridine-2-nonanoic acid, 8,8-difluoro-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



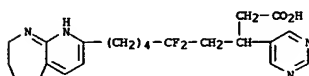
RN 393177-93-0 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 8,8-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



RN 393177-94-1 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-8,8-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



RN 393177-95-2 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 8,8-difluoro-5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)- (9CI) (CA INDEX NAME)

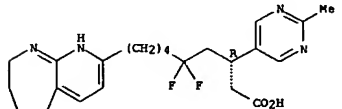


RN 393177-96-3 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 8,8-difluoro-5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (8S)- (9CI) (CA INDEX NAME)

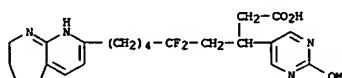
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

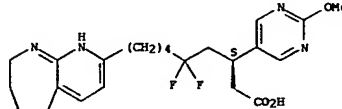


RN 393178-01-3 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 8,8-difluoro-5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



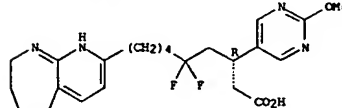
RN 393178-02-4 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 8,8-difluoro-5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393178-03-5 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 8,8-difluoro-5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, (8R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

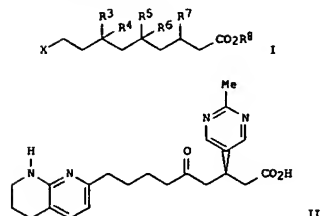
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:861451 CAPLUS  
 DOCUMENT NUMBER: 134:29136  
 TITLE: Novel nonanoic acid derivatives as alpha V integrin receptor antagonists  
 INVENTOR(S): Coleman, Paul J.; Duggan, Mark E.; Halczenko, Wasyl; Hartman, George D.; Hutchinson, John H.; Meissner, Robert S.; Patane, Michael A.; Perkins, James J.; Wang, Jiabing; Breslin, Michael J.  
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA  
 SOURCE: PCT Int. Appl., 166 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000072801	A2	20001207	WO 2000-US14901	20000530
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CH, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2373937	AA	20001207	CA 2000-2373937	20000530
BR 2000011108	A	20020319	BR 2000-11108	20000530
EP 1187592	A2	20020320	EP 2000-942652	20000530
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
TR 200103431	T2	20020621	TR 2001-200103431	20000530
AU 749351	B2	20020627	AU 2000-57246	20000530
EE 200100642	A	20030217	EE 2001-642	20000530
JP 2004500326	T2	20040108	JP 2000-620913	20000530
US 6410526	B1	20020625	US 2000-583522	20000531
ZA 2001009837	A	20040310	ZA 2001-9837	20011129
NO 2001005858	A	20020204	NO 2001-5858	20011130
HR 2001000895	A1	20030831	HR 2001-895	20011130
BG 106232	A	20020628	BG 2001-106232	20011218
PRIORITY APPLN. INFO.:			US 1999-137101P	P 19990602
OTHER SOURCE(S):	MARPAT 134:29136		US 2000-179216P	P 20000131
GI			WO 2000-US14901	W 20000530

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB The invention discloses novel nonanoic acid derivs. I [X = substituted pyridine, pyrimidine, naphthyridine, etc; R3, R5 = H, OH, alkoxy; R4, R6 = H, alkyl; R3 and R4 or R5 and R6 taken together may form carbonyl oxygen; R7 = (un)substituted Ph, naphthyl, pyridyl, furyl, thienyl, etc.; R8 = H, alkyl] as  $\alpha$ V integrin receptor antagonists along with methods for preparation. Thus, compound II was prepared in eight steps

from 6-oxo-heptanoic acid with chromatog. resolution of intermediate diketoester racemate. More particularly, the compds. of the present invention are antagonists of the integrin receptors  $\alpha$ v $\beta$ 3 and  $\alpha$ v $\beta$ 5, and are useful for inhibiting bone resorption, treating and preventing osteoporosis, and inhibiting vascular restenosis, diabetic retinopathy, macular degeneration, angiogenesis, atherosclerosis, inflammation, inflammatory arthritis, viral disease, cancer, and metastatic tumor growth.

IT 312261-73-7P 312261-74-8P 312262-00-3P  
 312262-01-4P 312262-03-6P 312262-04-7P  
 312262-06-9P 312262-07-0P 312262-09-2P  
 312262-10-5P 312262-12-7P 312262-13-8P  
 312262-15-0P 312262-16-1P 312262-21-8P  
 312262-22-9P 312262-24-1P 312262-25-2P  
 312262-35-4P 312262-36-5P

RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

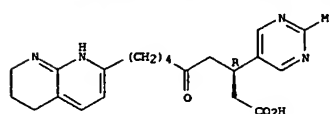
(Preparation and biol. activity of nonanoic acid derivs. as  $\alpha$ V integrin receptor antagonists)

RN 312261-73-7 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)- $\delta$ -oxo-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

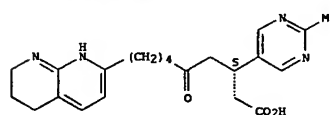
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 312261-74-8 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)- $\delta$ -oxo-, (BS)- (9CI) (CA INDEX NAME)

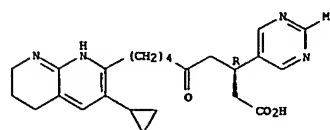
Absolute stereochemistry.



RN 312262-00-3 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)- $\delta$ -oxo-, (BR)- (9CI) (CA INDEX NAME)

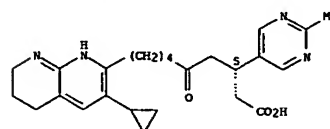
Absolute stereochemistry.



RN 312262-01-4 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)- $\delta$ -oxo-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

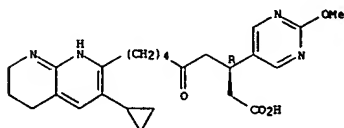


L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STM (Continued)

RN 312262-03-6 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro- $\beta$ -(2-methoxy-5-pyrimidinyl)- $\delta$ -oxo-, (BR)- (9CI) (CA INDEX NAME)

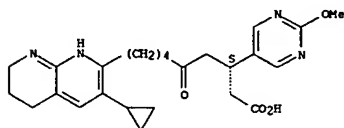
Absolute stereochemistry.



RN 312262-04-7 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro- $\beta$ -(2-methoxy-5-pyrimidinyl)- $\delta$ -oxo-, (BS)- (9CI) (CA INDEX NAME)

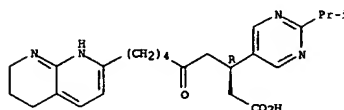
Absolute stereochemistry.



RN 312262-06-9 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -[2-(1-methylethyl)-5-pyrimidinyl]- $\delta$ -oxo-, (BR)- (9CI) (CA INDEX NAME)

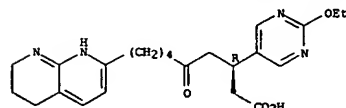
Absolute stereochemistry.



RN 312262-07-0 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -[2-(1-methylethyl)-5-pyrimidinyl]- $\delta$ -oxo-, (BS)- (9CI) (CA INDEX NAME)

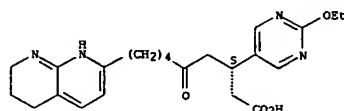
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STM (Continued)



RN 312262-13-8 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid,  $\beta$ -(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro- $\delta$ -oxo-, (BS)- (9CI) (CA INDEX NAME)

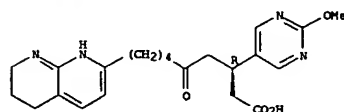
Absolute stereochemistry.



RN 312262-15-0 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methoxy-5-pyrimidinyl)- $\delta$ -oxo-, (BR)- (9CI) (CA INDEX NAME)

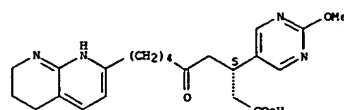
Absolute stereochemistry.



RN 312262-16-1 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methoxy-5-pyrimidinyl)- $\delta$ -oxo-, (BS)- (9CI) (CA INDEX NAME)

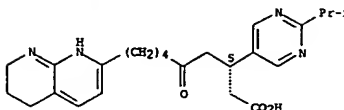
Absolute stereochemistry.



RN 312262-21-8 CAPLUS

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STM (Continued)

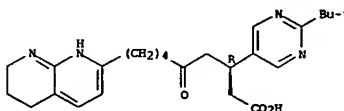
Absolute stereochemistry.



RN 312262-09-2 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid,  $\beta$ -[2-(1,1-dimethylethyl)-5-pyrimidinyl]-1,5,6,7-tetrahydro- $\delta$ -oxo-, (BR)- (9CI) (CA INDEX NAME)

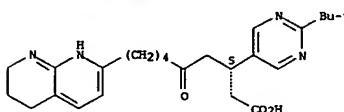
Absolute stereochemistry.



RN 312262-10-5 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid,  $\beta$ -[2-(1,1-dimethylethyl)-5-pyrimidinyl]-1,5,6,7-tetrahydro- $\delta$ -oxo-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312262-12-7 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid,  $\beta$ -(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro- $\delta$ -oxo-, (BR)- (9CI) (CA INDEX NAME)

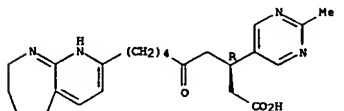
Absolute stereochemistry.



L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STM (Continued)

CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)- $\delta$ -oxo-, (BR)- (9CI) (CA INDEX NAME)

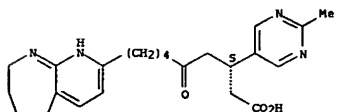
Absolute stereochemistry.



RN 312262-22-9 CAPLUS

CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)- $\delta$ -oxo-, (BS)- (9CI) (CA INDEX NAME)

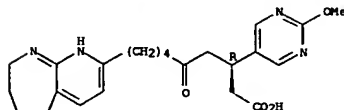
Absolute stereochemistry.



RN 312262-24-1 CAPLUS

CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro- $\beta$ -(2-methoxy-5-pyrimidinyl)- $\delta$ -oxo-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

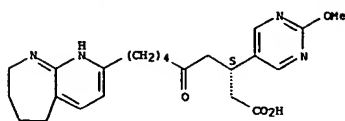


RN 312262-25-2 CAPLUS

CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro- $\beta$ -(2-methoxy-5-pyrimidinyl)- $\delta$ -oxo-, (BS)- (9CI) (CA INDEX NAME)

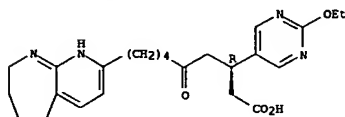
Absolute stereochemistry. Rotation (-).

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



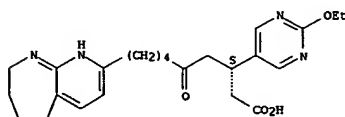
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CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid,  $\beta$ -(2-ethoxy-5-pyrimidinyl)-5,6,7,8-tetrahydro-8-oxo-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312262-36-5 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid,  $\beta$ -(2-ethoxy-5-pyrimidinyl)-5,6,7,8-tetrahydro-8-oxo-, (BS)- (9CI) (CA INDEX NAME)

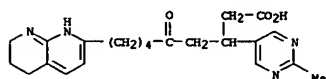
Absolute stereochemistry.



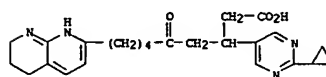
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L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 312261-72-6 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro- $\beta$ -(2-methyl-5-pyrimidinyl)-8-oxo-, (9CI) (CA INDEX NAME)

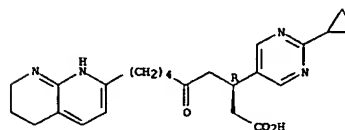


RN 312261-75-9 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid,  $\beta$ -(2-cyclopropyl-5-pyrimidinyl)-1,5,6,7-tetrahydro-8-oxo-, (9CI) (CA INDEX NAME)



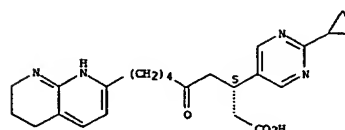
RN 312261-76-0 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid,  $\beta$ -(2-cyclopropyl-5-pyrimidinyl)-1,5,6,7-tetrahydro-8-oxo-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312261-77-1 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid,  $\beta$ -(2-cyclopropyl-5-pyrimidinyl)-1,5,6,7-tetrahydro-8-oxo-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



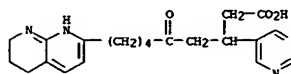
RN 312261-78-2 CAPLUS

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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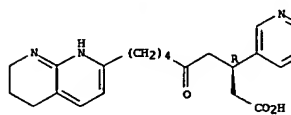
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and biol. activity of nonanoic acid derivs. as  $\alpha$  integrin receptor antagonists)

RN 312261-69-1 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-8-oxo- $\beta$ -5-pyrimidinyl-, (9CI) (CA INDEX NAME)



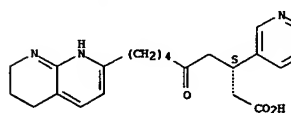
RN 312261-70-4 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-8-oxo- $\beta$ -5-pyrimidinyl-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



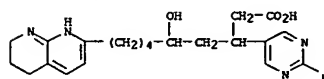
RN 312261-71-5 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-8-oxo- $\beta$ -5-pyrimidinyl-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



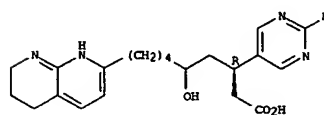
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 312261-79-3 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-8-hydroxy- $\beta$ -(2-methyl-5-pyrimidinyl)-8-oxo-, (9CI) (CA INDEX NAME)



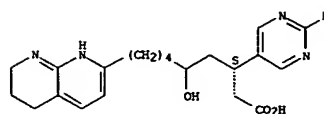
RN 312261-79-3 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-8-hydroxy- $\beta$ -(2-methyl-5-pyrimidinyl)-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

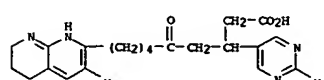


RN 312261-80-6 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-8-hydroxy- $\beta$ -(2-methyl-5-pyrimidinyl)-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

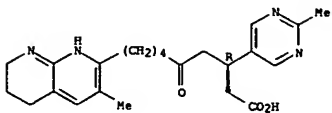


RN 312261-81-7 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-3-methyl- $\beta$ -(2-methyl-5-pyrimidinyl)-8-oxo-, (9CI) (CA INDEX NAME)



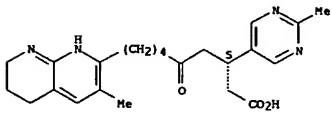
RN 312261-82-8 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-3-methyl- $\beta$ -(2-methyl-5-pyrimidinyl)-8-oxo-, (BR)- (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 Absolute stereochemistry.

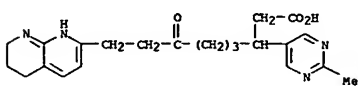


RN 312261-83-9 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-3-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (PS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

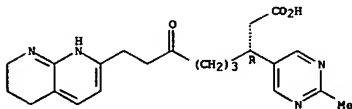


RN 312261-84-0 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-ζ-oxo-, (9CI) (CA INDEX NAME)

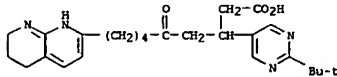


RN 312261-85-1 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-ζ-oxo-, (BR)- (9CI) (CA INDEX NAME)

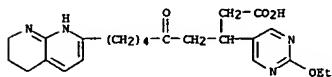
Absolute stereochemistry.



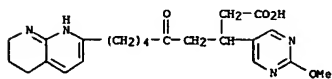
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



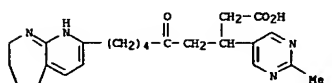
RN 312262-11-6 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, β-(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo-, (9CI) (CA INDEX NAME)



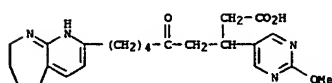
RN 312262-14-9 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (9CI) (CA INDEX NAME)



RN 312262-20-7 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (9CI) (CA INDEX NAME)



RN 312262-23-0 CAPLUS  
 CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (9CI) (CA INDEX NAME)

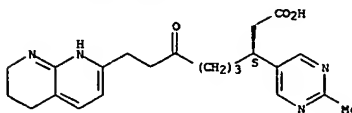


RN 312262-29-6 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, β-[6-[6-(methylamino)-2-pyridinyl]-2-oxohexyl]- (9CI) (CA INDEX NAME)

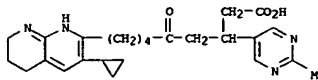
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 312261-86-2 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-ζ-oxo-, (PS)- (9CI) (CA INDEX NAME)

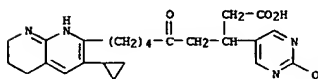
Absolute stereochemistry.



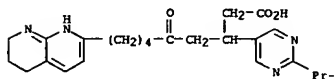
RN 312261-99-7 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (9CI) (CA INDEX NAME)



RN 312262-02-5 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (9CI) (CA INDEX NAME)



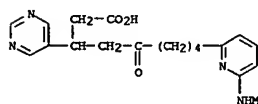
RN 312262-05-8 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-[2-(1-methylethyl)-5-pyrimidinyl]-δ-oxo-, (9CI) (CA INDEX NAME)



RN 312262-08-1 CAPLUS  
 CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(1,1-dimethylethyl)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo-, (9CI) (CA INDEX NAME)

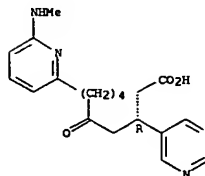
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

oxohexyl]- (9CI) (CA INDEX NAME)



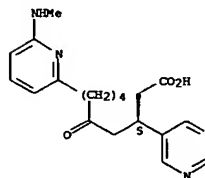
RN 312262-30-9 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, β-[6-[6-(methylamino)-2-pyridinyl]-2-oxohexyl]-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



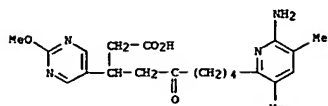
RN 312262-31-0 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, β-[6-[6-(methylamino)-2-pyridinyl]-2-oxohexyl]-, (PS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

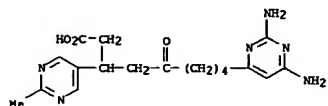


RN 312262-32-1 CAPLUS  
 CN 5-Pyrimidinepropanoic acid, β-[6-[6-(6-amino-3,5-dimethyl-2-pyridinyl)-2-oxohexyl]-2-methoxy-, (9CI) (CA INDEX NAME)

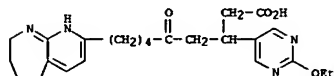
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



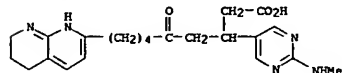
RN 312262-33-2 CAPLUS  
CN 4-Pyridinononanoic acid, 2,6-diamino-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-34-3 CAPLUS  
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, β-(2-ethoxy-5-pyrimidinyl)-5,6,7,8-tetrahydro-δ-oxo- (9CI) (CA INDEX NAME)

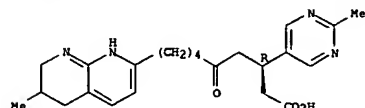


RN 312262-46-7 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methylamino)-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



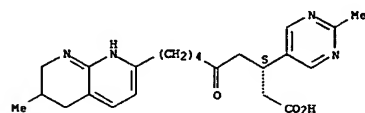
RN 312262-47-8 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methylamino)-5-pyrimidinyl)-δ-oxo-, (BR)- (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

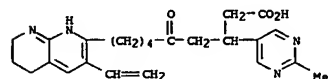


RN 312262-54-7 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-6-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (PS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

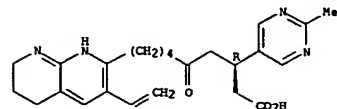


RN 312262-61-6 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-ethenyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-62-7 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-ethenyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (BR)- (9CI) (CA INDEX NAME)

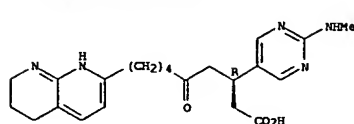
Absolute stereochemistry.



RN 312262-63-8 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-ethenyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (PS)- (9CI) (CA INDEX NAME)

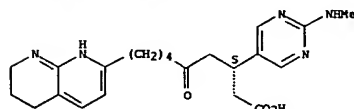
Absolute stereochemistry.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

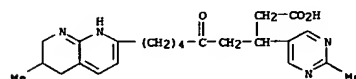


RN 312262-48-9 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methylamino)-5-pyrimidinyl)-δ-oxo-, (PS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



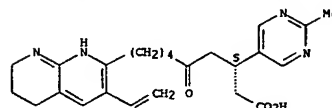
RN 312262-52-5 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-6-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



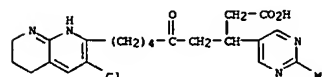
RN 312262-53-6 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-6-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

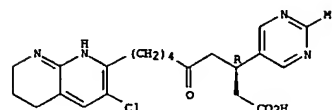


RN 312262-64-9 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-chloro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



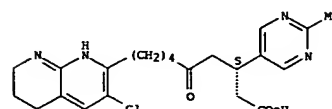
RN 312262-65-0 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-chloro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



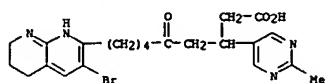
RN 312262-66-1 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-chloro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (PS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



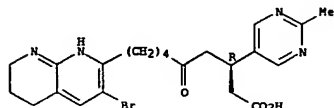
RN 312262-67-2 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-bromo-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



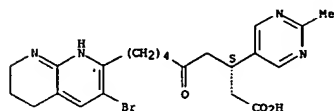
RN 312262-68-3 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-bromo-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (BR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

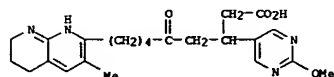


RN 312262-69-4 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-bromo-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (BS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

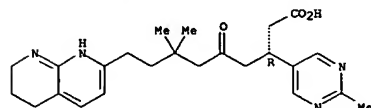


RN 312262-70-7 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-3-methyl-δ-oxo- (9CI) (CA INDEX NAME)



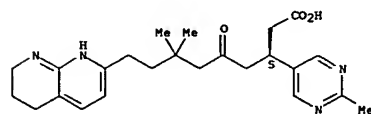
RN 312262-71-8 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (BR) - (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

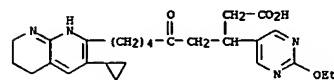


RN 312262-78-5 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (BS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

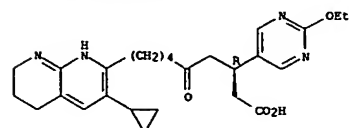


RN 312262-79-6 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-β-(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo- (9CI) (CA INDEX NAME)



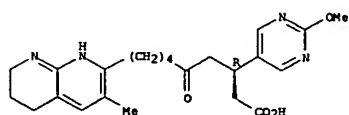
RN 312262-80-9 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-β-(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo-, (BR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



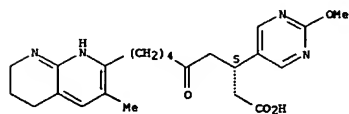
RN 312262-81-0 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-β-(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo-, (BS) - (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

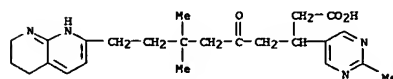


RN 312262-72-9 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (BS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



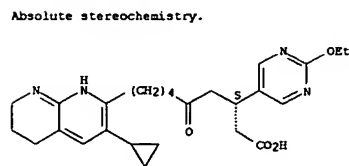
RN 312262-76-3 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



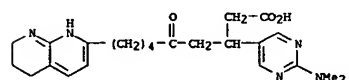
RN 312262-77-4 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (BR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

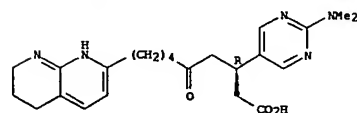


RN 312262-85-4 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(dimethylamino)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo- (9CI) (CA INDEX NAME)



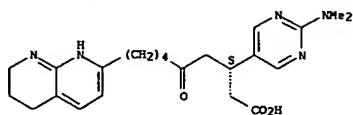
RN 312262-86-5 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(dimethylamino)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo-, (BR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



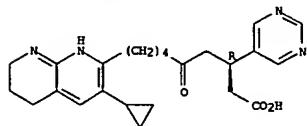
RN 312262-87-6 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(dimethylamino)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo-, (BS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



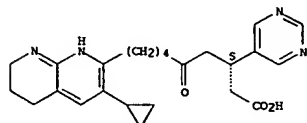
RN 312262-88-7 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-8-oxo-β-5-pyrimidinyl-, (BR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312262-89-8 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-8-oxo-β-5-pyrimidinyl-, (BS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312263-62-0 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-3-methyl-8-oxo-, (BR)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

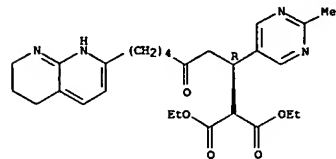
CRN 312262-71-8  
CMF C23 H30 N4 O4

Absolute stereochemistry.

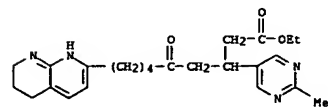


IT 312262-91-2P 312262-92-3P 312262-95-6P  
312262-96-7P 312262-97-8P 312263-01-7P  
312263-02-8P 312263-09-5P 312263-10-8P  
312263-17-7P 312263-28-8P 312263-29-9P  
312263-30-2P 312263-31-3P 312263-33-5P  
312263-34-6P 312263-35-7P 312263-42-6P  
312263-43-7P 312263-52-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and biol. activity of nonanoic acid derivs. as αv integrin receptor antagonists)  
RN 312262-91-2 CAPLUS  
CN Propanediolic acid, [(1R)-1-(2-methyl-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

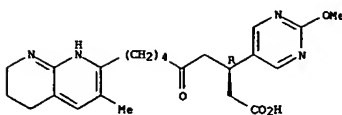
Absolute stereochemistry.



RN 312262-92-3 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-8-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 312262-95-6 CAPLUS  
CN 5-Pyrimidinepropanoic acid, β-ethenyl-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)



CH 2

CRN 76-05-1  
CMF C2 H F3 O2

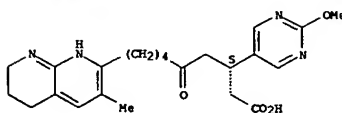


RN 312263-63-1 CAPLUS  
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-3-methyl-8-oxo-, (BS)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

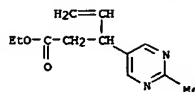
CRN 312262-72-9  
CMF C23 H30 N4 O4

Absolute stereochemistry.

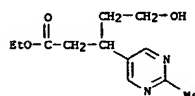


CH 2

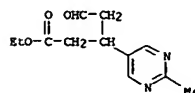
CRN 76-05-1  
CMF C2 H F3 O2



RN 312262-96-7 CAPLUS  
CN 5-Pyrimidinepropanoic acid, β-(2-hydroxyethyl)-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

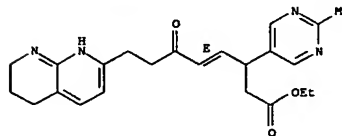


RN 312262-97-8 CAPLUS  
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-(2-oxoethyl)-, ethyl ester (9CI) (CA INDEX NAME)

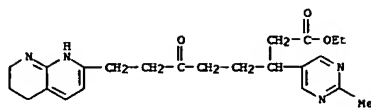


RN 312263-01-7 CAPLUS  
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[(1E)-3-oxo-5-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-pentenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

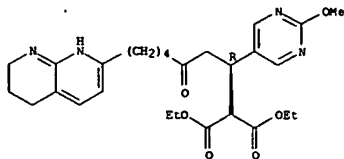


RN 312263-02-8 CAPLUS  
CN 1,8-Naphthyridine-2-octanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-8-oxo-, ethyl ester (9CI) (CA INDEX NAME)



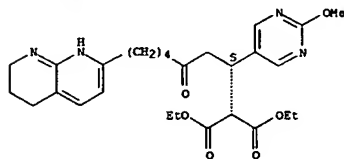
RN 312263-09-5 CAPLUS  
CN Propanedioic acid, [(1R)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

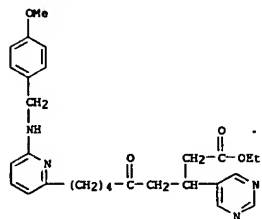


RN 312263-10-8 CAPLUS  
CN Propanedioic acid, [(1S)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

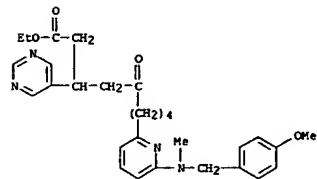
Absolute stereochemistry.



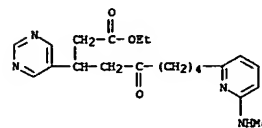
RN 312263-27-7 CAPLUS  
CN Propanedioic acid, [(1S)-7-[6-[[[(4-methoxyphenyl)methyl]amino]-2-pyridinyl]-3-oxo-1-(5-pyrimidinyl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)



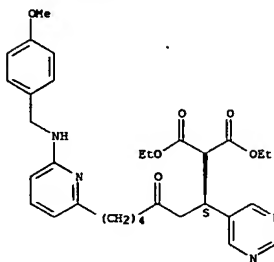
RN 312263-30-2 CAPLUS  
CN 5-Pyrimidinepropanoic acid, β-[6-[6-[[[(4-methoxyphenyl)methyl]amino]-2-pyridinyl]-2-oxohexyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 312263-31-3 CAPLUS  
CN 5-Pyrimidinepropanoic acid, β-[6-[6-(methylamino)-2-pyridinyl]-2-oxohexyl]-, ethyl ester (9CI) (CA INDEX NAME)

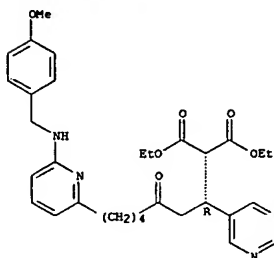


RN 312263-33-5 CAPLUS  
CN Propanedioic acid, [1-(2-methyl-5-pyrimidinyl)-3-oxo-6-heptenyl]-, diethyl ester (9CI) (CA INDEX NAME)

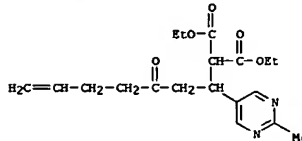


RN 312263-28-8 CAPLUS  
CN Propanedioic acid, [(1R)-7-[6-[[[(4-methoxyphenyl)methyl]amino]-2-pyridinyl]-3-oxo-1-(5-pyrimidinyl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

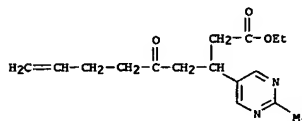
Absolute stereochemistry.



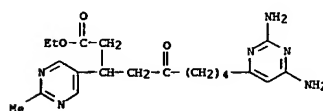
RN 312263-29-9 CAPLUS  
CN 5-Pyrimidinepropanoic acid, β-[6-[6-[[[(4-methoxyphenyl)methyl]amino]-2-pyridinyl]-2-oxohexyl]-, ethyl ester (9CI) (CA INDEX NAME)



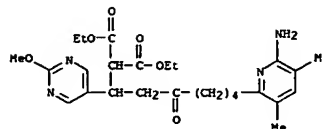
RN 312263-34-6 CAPLUS  
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-(2-oxo-5-hexenyl)-, ethyl ester (9CI) (CA INDEX NAME)



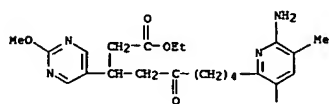
RN 312263-35-7 CAPLUS  
CN 4-Pyrimidinepropanoic acid, 2,6-diamino-β-(2-methyl-5-pyrimidinyl)-5-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 312263-42-6 CAPLUS  
CN Propanedioic acid, [7-(6-amino-3,5-dimethyl-2-pyridinyl)-1-(2-methoxy-5-pyrimidinyl)-3-oxoheptyl]-, diethyl ester (9CI) (CA INDEX NAME)

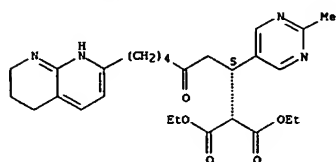


L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 RN 312263-43-7 CAPLUS  
 CN 5-Pyrimidinepropanoic acid,  $\beta$ -[6-(6-amino-3,5-dimethyl-2-pyridinyl)-2-oxohexyl]-2-methoxy-, ethyl ester (9CI) (CA INDEX NAME)



RN 312263-52-8 CAPLUS  
 CN Propanedioic acid, [(15)-1-(2-methyl-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

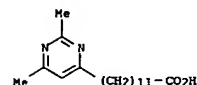
Absolute stereochemistry.



L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1954:32620 CAPLUS  
 DOCUMENT NUMBER: 48:32620  
 ORIGINAL REFERENCE NO.: 48:5865d-1,5866a  
 TITLE: Synthesis of potential antibacterial agents. II. A pyrimidine analog of chaalmoogric acid  
 AUTHOR(S): Heyes, T. D.; Roberts, John C.  
 SOURCE: Journal of the Chemical Society, Abstracts (1952) 4935-7  
 CODEN: JCSAA2; ISSN: 0590-9791

DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 48:32620  
 AB cf. C.A. 45, 3332d. A general synthesis for  $\alpha$ -(2,6-dimethyl-4-pyrimidyl)alkane-1-carboxylic acids has been devised. Attempts to prepare  $\alpha$ -(2-pyrimidyl)- and  $\alpha$ -(5-pyrimidyl)alkane-1-carboxylic acids failed. Br(CH<sub>2</sub>)<sub>10</sub>CO<sub>2</sub>Et (I) (14.6 g.), 13 g. KCN, 100 cc. EtOH, and 20 cc. H<sub>2</sub>O refluxed 3 hrs., cooled, shaken with H<sub>2</sub>O, the insol. part dissolved in Et<sub>2</sub>O, the Et<sub>2</sub>O washed with H<sub>2</sub>O, dried (Na<sub>2</sub>SO<sub>4</sub>), and filtered; removal of Et<sub>2</sub>O and distillation in vacuo gave Et 10-cyano-1-decanecarboxylate (II),  
 b11 196-8°. Dry HCl was passed into 5 g. II and 1 g. dry ice-cooled EtOH until 8.2 g. was absorbed, the mixture left at room temperature 14 hrs., 5 cc. Et<sub>2</sub>O added, the precipitated Et imidate-HCl filtered, dissolved in 15 cc. dry EtOH, dry 9% NH<sub>3</sub>-EtOH (50 cc.) added, the mixture shaken for 1 hr. then concentrated, the NH<sub>4</sub>Cl removed the filtrate evaporated, and the residue dissolved in O(CH<sub>2</sub>CH<sub>2</sub>OH)<sub>2</sub>, dry ether added, and the precipitate crystallized from C<sub>6</sub>H<sub>6</sub>, giving 2.0 g. 11-carbomethoxyundecanamide-HCl (III) as waxlike plates, m. 79°. III (1 g.) in 10 cc. EtOH added to 0.3 g. CH<sub>2</sub>Ac<sub>2</sub> and 0.8 g. NaOEt in 15 cc. dry EtOH, the mixture kept 6 days at room temperature, diluted with 20 cc. H<sub>2</sub>O refluxed 1 hr., diluted with H<sub>2</sub>O, acidified, filtered, and the precipitate crystallized from aqueous EtOH gave 0.7 g. of 10-carbamoyl-1-decanecarboxylic acid (IV), prisms, m. 143°. Me H sebacate (20 g.) added to 60 g. SOC1<sub>2</sub> and refluxed 4 hrs. yielded 9-carbomethoxyundecanoyl chloride (V), b23 177°. To 7.14 g. PhLi in 150 cc. dry Et<sub>2</sub>O under N was added with stirring 10.4 g. 2,4,6-trimethylpyrimidine (VI) in 50 cc. dry Et<sub>2</sub>O, the mixture refluxed and stirred 15 min., treated with 18 g. V in 50 cc. dry Et<sub>2</sub>O, refluxed and stirred 3 hrs., let stand overnight under N, shaken with H<sub>2</sub>O, the Et<sub>2</sub>O layer extracted with 2N HCl, the acid exts. were made alkaline, extracted with Et<sub>2</sub>O, the exts. dried with MgSO<sub>4</sub>, filtered, the residue was refluxed 2.5 hrs. with 50 cc. 10% KOH in EtOH, diluted with H<sub>2</sub>O, extracted with Et<sub>2</sub>O, the aqueous layer was raised to pH 6.5, the emulsion extracted with Et<sub>2</sub>O, the extract dried, filtered, evaporated, the residue extracted with hot petroleum (b. 100-20°). Cooling gave 0.05 g. crystals which were heated with C in MeOH and filtered; evaporation of the solvent and crystallization of the residue from light petroleum gave tan needles, to a solution of which in

L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 C<sub>6</sub>H<sub>6</sub> was added light petroleum (b. 60-80°) to turbidity, and the first yellow ppt. filtered off; addn. of more light petroleum pptd. 8.5 mg. 10-(2,6-dimethyl-4-pyrimidyl)-9-oxo-1-decanecarboxylic acid (VII), prisms, m. 96-7°. Similarly 2,6-dimethyl-4-pyrimidylmethyl lithium heated with 10-bromo-1-decanecarboxylate, hydrolyzed, and treated with HCl gave 11-(2,6-dimethyl-4-pyrimidyl)-1-undecanecarboxylic acid (VIII), m. 94° (tuberculostatic activity of 1). 1-Bromodecanecarboxylic acid (22 g.) was refluxed with 19 cc. SOC1<sub>2</sub> 1 hr. and the excess of the reagent removed in vacuo; distn. gave a fraction (14.7 g.), b16 186°, which was added in 50 cc. dry Et<sub>2</sub>O during 15 min. at 0-5° to CH<sub>2</sub>N<sub>2</sub> [from 30 g. MeN(NO)CONH<sub>2</sub>] in Et<sub>2</sub>O, the mixt. was kept at room temp. 1 hr., then evapd. in vacuo at 25°, the solid residue heated in 100 cc. dry EtOH to 55-60°, 6.8 g. dry Ag<sub>2</sub>O in 30 cc. dry EtOH added in portions, and the mixt. raised to b.p. and filtered; distn. gave 7 g. impure ethyl Br(CH<sub>2</sub>)<sub>11</sub>CO<sub>2</sub>Et (IX). Isolated, hydrolyzed, and purified as described for VII to give platelets of 12-(2,6-dimethyl-4-pyrimidyl)-1-dodecanecarboxylic acid m. 96.5° [tuberculostatic activity 5 (loc. cit.)].  
 IT 057412-52-3, 4-Pyrimidinedodecanoic acid, 2,6-dimethyl-  
 057412-61-4, 4-Pyrimidinetridecanoic acid, 2,6-dimethyl-  
 (preparation of)  
 RN 057412-52-3 CAPLUS  
 CN 4-Pyrimidinedodecanoic acid, 2,6-dimethyl- (5CI) (CA INDEX NAME)



RN 057412-61-4 CAPLUS  
 CN 4-Pyrimidinetridecanoic acid, 2,6-dimethyl- (5CI) (CA INDEX NAME)

